09/934,972

(FILE 'HOME' ENTERED AT 15:32:35 ON 27 APR 2005)

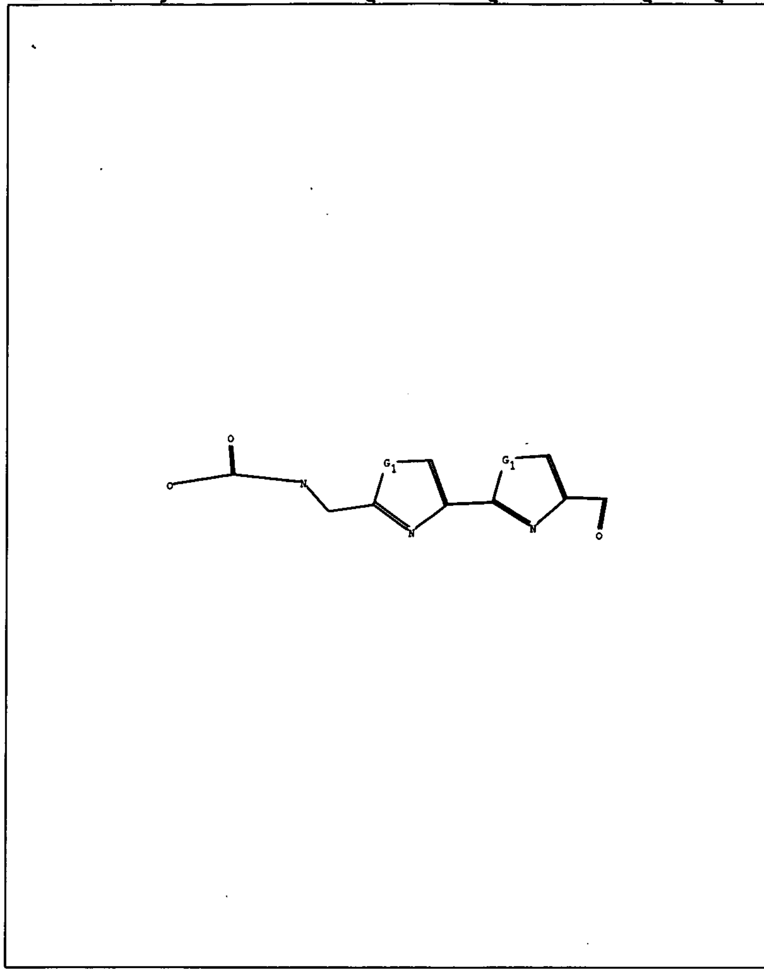
FILE 'REGISTRY' ENTERED AT 15:33:28 ON 27 APR 2005
L1 STRUCTURE UPLOADED

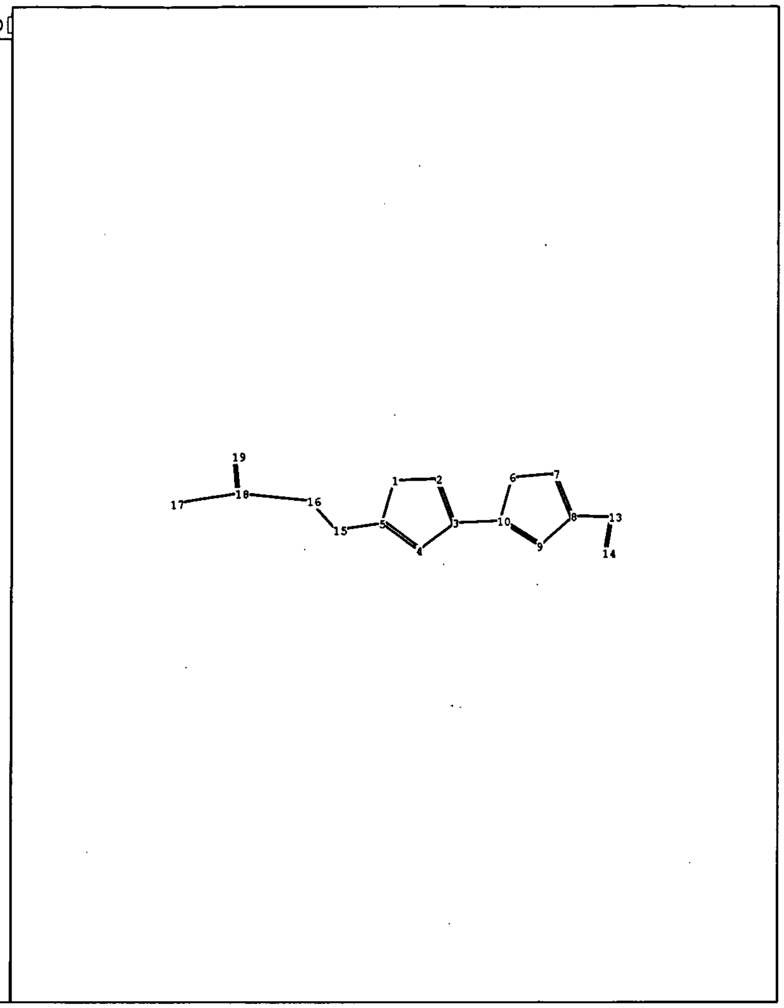
FILE 'STNGUIDE' ENTERED AT 15:33:58 ON 27 APR 2005

FILE 'REGISTRY' ENTERED AT 15:34:23 ON 27 APR 2005
L2 25 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:35:05 ON 27 APR 2005
L3 13 S L2

=>





chain nodes :
13 14 15 16 17 18 19

ring nodes :
1 2 3 4 5 6 7 8 9 10

chain bonds :
3-10 5-15 8-13 13-14 15-16 16-18 17-18 18-19

ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10

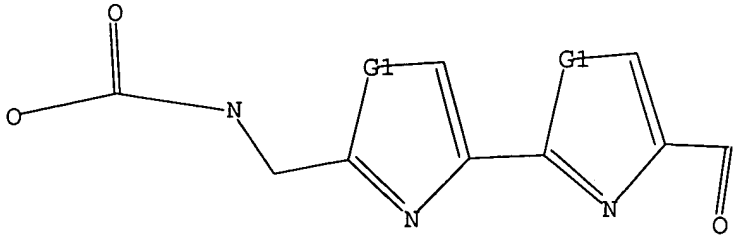
exact/norm bonds :
1-2 1-5 2-3 3-4 3-10 4-5 5-15 6-7 6-10 7-8 8-9
8-13 9-10 13-14 15-16 16-18 17-18 18-19

G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom
8:Atom 9:Atom 10:Atom 13:CLASS 14:CLASS 15:CLASS
16:CLASS 17:CLASS 18:CLASS 19:CLASS

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

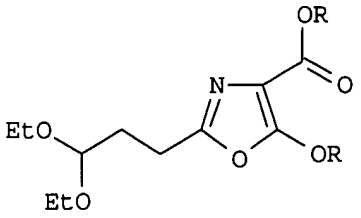
L3 ANSWER 10 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1999:648054 CAPLUS
DN 132:36007
ED Entered STN: 12 Oct 1999
TI Synthesis of thiazole, imidazole and oxazole containing amino acids for peptide backbone modification
AU Stankova, Ivanka G.; Videnov, Georgi I.; Golovinsky, Evgeny V.; Jung, Guenther
CS Department of Chemistry, Southwest University "N. Rilski", Blagoevgrad, 2700, Bulg.
SO Journal of Peptide Science (1999), 5(9), 392-398
CODEN: JPSIEI; ISSN: 1075-2617
PB John Wiley & Sons Ltd.
DT Journal
LA English
CC 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 28
AB Novel 5-membered heterocyclic ring-containing amino acid building blocks are synthesized. These can be incorporated into analogs of peptide antibiotics such as microcin B17, which is a potent DNA-gyrase inhibitor that exhibits eight thiazole and oxazole moieties. In particular, the syntheses of imidazole and bisoxazole amino acids as novel peptidomimetics are reported, this includes a new procedure for the oxidative conversion of the intermediates oxazoline, imidazoline as well as oxazole-oxazoline into the corresponding heteroarom. compds. A mixture of DBU/CCl4/MeCN and pyridine proved to be a very effective and mild agent for this oxidation step.
ST amino acid heterocyclic prepn peptidomimetic building block; thiazole contg amino acid prepn; imidazole contg amino acid prepn; oxazole contg amino acid prepn; DBU reagent oxazoline oxidn oxazole
IT Amino acids, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(heterocyclic; preparation of thiazole, imidazole and oxazole containing amino
acids useful for peptide synthesis)
IT Peptidomimetics
(preparation of thiazole, imidazole and oxazole containing amino acids as building blocks for peptidomimetics)
IT Peptides, preparation
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT Heterocyclic compounds
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 84286-90-8P, Microcin B17
RL: PNU (Preparation, unclassified); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 1113-59-3, 3-Bromo-2-oxopropanoic acid 1138-80-3 1668-10-6, H-Gly-NH2·HCl 5680-80-8, H-Ser-OMe·HCl 161372-39-0 200116-81-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 949-90-6P 1755-98-2P 35150-09-5P 182120-87-2P 252348-72-4P 252348-73-5P 252348-75-7P 252348-77-9P 252348-78-0P 252348-79-1P

252348-80-4P 252348-81-5P **252348-82-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
IT 252348-74-6P 252348-76-8P **252348-83-7P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of thiazole, imidazole and oxazole containing amino acids useful
for peptide synthesis)
RE.CNT 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Aguilar, E; Tetrahedron Lett 1994, V35, P2477 CAPLUS
(2) Anderson, M; J Chem Soc Perkin Trans 2 1986, P1995 CAPLUS
(3) Bayer, A; Angew Chem 1993, V105, P1410 CAPLUS
(4) Bayer, A; Angew Chem Int Ed Engl 1993, V32, P1336
(5) Bayer, A; Eur J Biochem 1995, V234, P414 CAPLUS
(6) Bayer, A; Proceedings of the 22nd European Peptide Symposium 1992, P117
(7) Bergeron, R; J Org Chem 1985, V50, P2780 CAPLUS
(8) Bergmann, M; Chem Ber 1932, V65(7), P1192
(9) Brenner, M; Helv Chim Acta 1953, V36, P1109 CAPLUS
(10) Drechsel, H; Liebigs Ann 1995, P1727 CAPLUS
(11) Fusetani, N; Chem Rev 1993, V93, P1793 CAPLUS
(12) Holzapfel, C; J Org Chem 1985, V50, P2323 CAPLUS
(13) Houssin, R; J Org Chem 1985, V50, P2787 CAPLUS
(14) Jones, R; Tetrahedron Lett 1988, V29, P3851
(15) Jung, G; Combinatorial Peptide and Non-Peptide Libraries 1996
(16) Kelly, R; J Org Chem 1986, V51, P4590 CAPLUS
(17) Mayers, A; Tetrahedron Lett 1994, V35, P2481
(18) Michael, J; Angew Chem Int Ed Engl 1993, V105, P1 CAPLUS
(19) Michael, J; Angew Chem Int Ed Engl 1993, V32, P1
(20) Pattenden, G; J Heterocyclic Chem 1992, V29, P607 CAPLUS
(21) Pozdnev, V; Tetrahedron Lett 1995, V36, P7115 CAPLUS
(22) Reuman, M; Tetrahedron 1985, V41, P837 CAPLUS
(23) Rondu, F; J Med Chem 1997, V40, P3793 CAPLUS
(24) Scheibye, S; Bull Soc Chim Belg 1978, V87, P229 CAPLUS
(25) Schmidt, U; Synthesis 1987, P233 CAPLUS
(26) Schmidt, U; Tetrahedron Lett 1986, V27, P163 CAPLUS
(27) Videnov, G; Angew Chem 1996, V108, P1604
(28) Videnov, G; Angew Chem 1996, V108, P1607
(29) Videnov, G; Angew Chem Int Ed Engl 1996, V35, P1503 CAPLUS
(30) Videnov, G; Angew Chem Int Ed Engl 1996, V35, P1506 CAPLUS
(31) Vorbrueggen, H; Tetrahedron 1993, V49, P9353 CAPLUS
(32) Wipf, P; J Org Chem 1993, V58, P3604 CAPLUS
(33) Yokoyama, M; Synthesis 1994, V3, P1467
(34) Yonetani, K; Bull Chem Soc Jpn 1975, V48, P3302 CAPLUS
(35) Zhi Ling, Y; J Med Chem 1997, V40, P3297

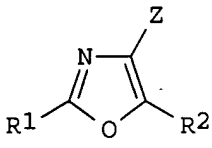
L3 ANSWER 11 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1998:120827 CAPLUS
DN 128:204827
ED Entered STN: 28 Feb 1998
TI Synthesis of functionalized oxazoles and bis-oxazoles
AU Bagley, Mark C.; Buck, Richard T.; Hind, S. Lucy; Moody, Christopher J.
CS Dep. Chem., Univ. Exeter, Exeter, Devon, EX4 4QD, UK
SO Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1998), (3), 591-600
CODEN: JCPRB4; ISSN: 0300-922X
PB Royal Society of Chemistry
DT Journal
LA English
CC 28-6 (Heterocyclic Compounds (More Than One Hetero Atom))

OS CASREACT 128:204827

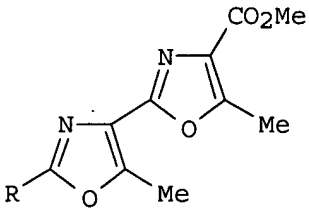
GI



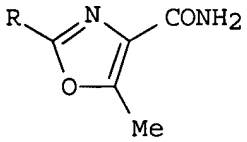
I



II



III



IV

AB A new method for the synthesis of oxazoles, and in particular chiral non-racemic oxazoles derived from amino acids, has been developed. Thus, rhodium(II) catalyzed reaction of diazocarbonyl compds. RO2CC(CO2R):N2 (R = Me, CMe3) and R2COCZ:N2 (R2 = Me, CH2Cl, Et, Ph, Z = CO2Me, CO2Et) in the presence of amides (EtO)2CHCH2CH2CONH2 and R1CONH2 [R1 = CbzNHCH2, (S)-BocNHCHCHMe2, (S)-CbzNHCHMe, etc.] results in regioselective insertion of the carbenoid into the amide N-H bond with formation of the β-carbonyl amides (EtO)2CH(CH2)2CONHCH(CO2R)2 and R2COCHZNHCOR1, resp. Cyclodehydration of these amides using triphenylphosphine-iodine-triethylamine gives functionalized oxazoles I and II. II [R1 = (S)-CbzNHCHCHMe2, (S)-N-Cbz-pyrrolidin-2-yl, R2 = Me, Z = CO2Me] were converted into the bis-oxazoles III by a second rhodium(II) catalyzed regioselective N-H insertion reaction on the amides IV, followed by cyclodehydration.

ST oxazole prepn; bisoxazole prepn

IT 1138-80-3 1142-20-7 1148-11-4 1149-26-4 6306-54-3 13734-41-3 18381-45-8 25275-28-9
RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of oxazoles and bis-oxazoles)

IT 949-90-6P 2624-36-4P 6773-29-1P, Dimethyl diazomalonate 13139-27-0P 13139-28-1P 24762-04-7P 28383-65-5P 34079-31-7P 35150-08-4P 35207-75-1P, Di-tert-butyl diazomalonate 104034-82-4P 182866-61-1P 182866-62-2P 182866-63-3P 182866-64-4P 182866-65-5P 182866-66-6P 182866-67-7P 182866-68-8P 182866-71-3P 182866-72-4P 182866-73-5P 182866-74-6P 182866-75-7P 182866-76-8P 203782-20-1P 203782-26-7P 203782-27-8P 203782-28-9P 203782-29-0P 203782-30-3P 203782-31-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of oxazoles and bis-oxazoles)

IT 182866-69-9P 182866-70-2P 203782-21-2P 203782-22-3P 203782-23-4P 203782-24-5P 203782-25-6P **203782-32-5P** 203782-33-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of oxazoles and bis-oxazoles)

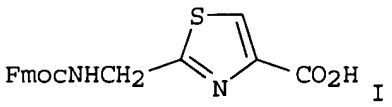
RE.CNT 65 THERE ARE 65 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

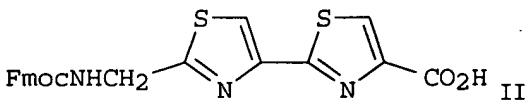
(1) Abernethy, J; Tetrahedron 1975, V31, P2659 CAPLUS
(2) Adams, J; Tetrahedron 1991, V47, P1765 CAPLUS
(3) Aguilar, E; Tetrahedron Lett 1994, V35, P2477 CAPLUS
(4) Aller, E; J Chem Soc, Perkin Trans 1 1996, P2879 CAPLUS

(5) Appel, R; Chem Ber 1983, V116, P2037 CAPLUS
(6) Bagley, M; Synlett 1996, P825 CAPLUS
(7) Baum, J; Synth Commun 1987, V17, P1709 CAPLUS
(8) Bianchi, M; Farmaco Ed Sci 1965, V20, P611 CAPLUS
(9) Boyd, G; Prog Heterocycl Chem 1996, V8, P192 CAPLUS
(10) Cama, L; Tetrahedron Lett 1978, V44, P4233
(11) Chattopadhyay, S; Tetrahedron Lett 1995, V36, P5271 CAPLUS
(12) Chen, S; Synthesis 1993, P858 CAPLUS
(13) Doyle, K; Synthesis 1994, P1021 CAPLUS
(14) Doyle, K; Tetrahedron 1994, V50, P3761 CAPLUS
(15) Doyle, M; Acc Chem Res 1986, V19, P348 CAPLUS
(16) Doyle, M; Chem Rev 1986, V86, P919 CAPLUS
(17) Evans, D; J Am Chem Soc 1992, V114, P9434 CAPLUS
(18) Ferris, L; J Chem Soc, Perkin Trans 1 1996, P2885 CAPLUS
(19) Garey, D; J Org Chem 1996, V61, P4853 CAPLUS
(20) Gilchrist, T; Contemp Org Synth 1994, V1, P205 CAPLUS
(21) Gilchrist, T; Contemp Org Synth 1995, V2, P337 CAPLUS
(22) Ibata, T; Bull Chem Soc Jpn 1992, V65, P3088 CAPLUS
(23) Ichiba, T; J Am Chem Soc 1991, V113, P3173 CAPLUS
(24) Ishibashi, Y; Tetrahedron Lett 1996, V37, P2997 CAPLUS
(25) Iwasaki, S; J Antibiol 1986, V39, P424 CAPLUS
(26) Jansen, R; Liebigs Ann Chem 1991, P707 CAPLUS
(27) Kato, Y; J Am Chem Soc 1986, V108, P2780 CAPLUS
(28) Khlebnikov, A; Adv Heterocycl Chem 1996, V65, P93 CAPLUS
(29) Knight, D; Synlett 1990, P36 CAPLUS
(30) Koskinen, A; J Chem Soc, Chem Commun 1990, P652 CAPLUS
(31) Koyama, Y; Agric Biol Chem 1981, V45, P1285 CAPLUS
(32) Kunze, B; J Antibiot 1992, V45, P1549 CAPLUS
(33) Lee, J; Synth Commun 1995, V25, P1511 CAPLUS
(34) Lewis, J; Nat Prod Rep 1992, V9, P81 CAPLUS
(35) Lewis, J; Nat Prod Rep 1993, V10, P29 CAPLUS
(36) Lewis, J; Nat Prod Rep 1994, V11, P395 CAPLUS
(37) Lewis, J; Nat Prod Rep 1995, V12, P135 CAPLUS
(38) Lewis, J; Nat Prod Rep 1996, V13, P435 CAPLUS
(39) Maas, G; Top Curr Chem 1987, V137, P75 CAPLUS
(40) Matsunaga, S; J Am Chem Soc 1986, V108, P847 CAPLUS
(41) Michael, J; Angew Chem, Int Ed Engl 1993, V32, P1
(42) Miller, D; Tetrahedron 1995, V51, P10811 CAPLUS
(43) Moody, C; Prog Heterocycl Chem 1997, V9, P1 CAPLUS
(44) Nagatsu, A; Tetrahedron Lett 1995, V36, P4097 CAPLUS
(45) Nakada, M; Tetrahedron Lett 1993, V34, P1039 CAPLUS
(46) Osipov, S; Tetrahedron Lett 1996, V37, P615 CAPLUS
(47) Padwa, A; Angew Chem, Int Ed Engl 1994, V33, P1797
(48) Padwa, A; Chem Rev 1991, V91, P263 CAPLUS
(49) Padwa, A; Tetrahedron 1992, V48, P5385 CAPLUS
(50) Panek, J; J Org Chem 1996, V61, P6496 CAPLUS
(51) Pattenden, G; J Heterocycl Chem 1992, V29, P607 CAPLUS
(52) Pattenden, G; Personal communication
(53) Regitz, M; Diazo Compounds Properties and Synthesis 1986
(54) Roesener, J; J Am Chem Soc 1986, V108, P846 CAPLUS
(55) Shapiro, E; Russ Chem Rev 1993, V62, P447
(56) Tanimoto, N; Angew Chem, Int Ed Engl 1994, V33, P673
(57) Tavecchia, P; Tetrahedron 1995, V51, P4867 CAPLUS
(58) Todorova, A; J Org Chem 1995, V60, P7891 CAPLUS
(59) Wipf, P; Chem Rev 1995, V95, P2115 CAPLUS
(60) Wipf, P; J Am Chem Soc 1995, V117, P558 CAPLUS
(61) Wipf, P; J Org Chem 1993, V58, P3604 CAPLUS
(62) Wipf, P; J Org Chem 1996, V61, P6517 CAPLUS
(63) Wunsch, E; Chem Ber 1971, V104, P2430 MEDLINE
(64) Ye, T; Chem Rev 1994, V94, P1091 CAPLUS
(65) Zaragoza, F; Tetrahedron 1997, V53, P3425 CAPLUS

AN 1996:639425 CAPLUS
DN 125:329404
ED Entered STN: 30 Oct 1996
TI Synthesis of all-thiazole microcin B17
AU Videnov, G.; Ihlenfeldt, H. G.; Bayer, A.; Jung, G.
CS Institut fur Organische Chemie, Universitat Tubingen, Tuebingen, D-72076, Germany
SO Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga, Port., Sept. 4-10, 1994 (1995), Meeting Date 1994, 351-352. Editor(s): Maia, Hernani L. S. Publisher: ESCOM, Leiden, Neth.
CODEN: 63MBAO
DT Conference
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
GI



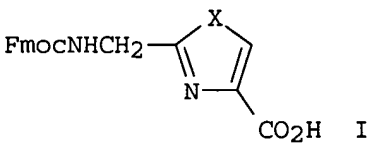
I



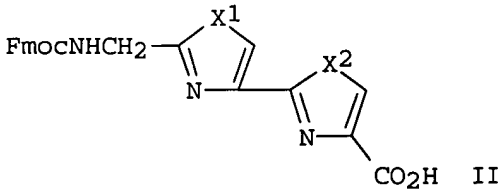
II

AB A report from a symposium on the solid-phase preparation of a microcin B17 analog in which all the oxazole rings are replaced with thiazole rings using thiazole and thoiazolylthiazole building blocks I and II (Fmoc = 9-fluorenylmethoxycarbonyl).
ST Merrifield synthesis thiazole microcin B17 symposium
IT Merrifield synthesis
(solid-phase preparation of all-thiazole microcin B17)
IT 182120-85-0P **182120-86-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(solid-phase preparation of all-thiazole microcin B17)
IT 84286-90-8DP, Microcin B17, all-thiazole analog 183270-54-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(solid-phase preparation of all-thiazole microcin B17)

L3 ANSWER 13 OF 13 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:473413 CAPLUS
DN 125:248418
ED Entered STN: 10 Aug 1996
TI Synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics
AU Videnov, Georgi; Kaiser, Dietmar; Kempter, Christoph; Jung, Guenther
CS Dipl.-Chem. C. Kempter, Inst. Organische Chemie Universitaet, Tuebingen, D-72076, Germany
SO Angewandte Chemie, International Edition in English (1996), 35(13/14), 1503-1506
CODEN: ACIEAY; ISSN: 0570-0833
PB VCH
DT Journal
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 28
OS CASREACT 125:248418
GI



I



II

AB Oxazole- and thiazole-containing peptides I (X = O, S) and II (X1, X2 = O, S) were prepared starting from glycinamide. Oxidative conversion of intermediate oxazoline into corresponding oxazole was carried out using DBU.

ST peptide mimetic oxazole thiazole

IT Peptides, preparation
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 1113-59-3 1668-10-6, Glycinamide hydrochloride 5680-80-8
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 35150-09-5P 71904-80-8P 89226-13-1P 182120-82-7P 182120-83-8P
182120-84-9P 182120-87-2P 182120-88-3P 182120-89-4P
182120-90-7P 182120-92-9P 182120-93-0P **182120-94-1P**
182120-95-2P 182120-97-4P 182120-98-5P **182120-99-6P**
182121-00-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

IT 182120-85-0P **182120-86-1P** 182120-91-8P **182120-96-3P**
182121-01-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of naturally occurring, conformationally restricted oxazole- and thiazole-containing di- and tripeptide mimetics)

=>

09/934,972

(FILE 'HOME' ENTERED AT 15:41:25 ON 27 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:41:35 ON 27 APR 2005

L1 STRUCTURE UPLOADED

L2 57 S L1 SSS FULL

FILE 'CAPLUS' ENTERED AT 15:42:20 ON 27 APR 2005

L3 80 S L2

L4 3 S L3 AND LIBRAR?

L5 77 S L3 NOT L4

L6 77 DUP REM L5 (0 DUPLICATES REMOVED)

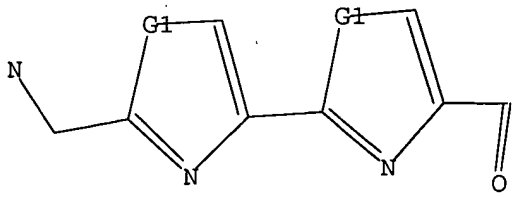
L7 77 S L6

L8 45 S L6 AND PEPTID?

L9 2 S L8 AND COMBINAT?

HAS NO ANSWERS

L1 STR



G1 O,S

09/936,972

(FILE 'HOME' ENTERED AT 15:04:23 ON 27 APR 2005)

FILE 'REGISTRY' ENTERED AT 15:04:40 ON 27 APR 2005

L1 STRUCTURE UPLOADED

L2 1 S L1

FILE 'STNGUIDE' ENTERED AT 15:07:59 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:14:01 ON 27 APR 2005

L3 11526 S (MARTIN, L? OR MARTIN L?)/AU,IN

L4 4515 S (HU, B? OR HU B?)/AU,IN

L5 9 S L3 AND L4

L6 6 DUP REM L5 (3 DUPLICATES REMOVED)

FILE 'STNGUIDE' ENTERED AT 15:16:54 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:20:35 ON 27 APR 2005

L7 3923 S OXAZOLE? AND THIAZOL?

L8 16 S L7 AND PEPTIDOMIMET?

L9 13 DUP REM L8 (3 DUPLICATES REMOVED)

L10 6826 S (JUNG, G? OR JUNG G?)/AU,IN

L11 31 S L10 AND OXAZOL?

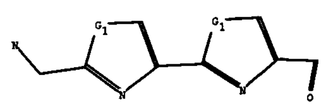
L12 25 S L11 AND THIAZOL?

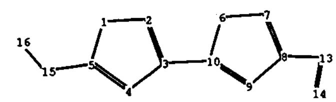
L13 14 DUP REM L12 (11 DUPLICATES REMOVED)

FILE 'STNGUIDE' ENTERED AT 15:25:10 ON 27 APR 2005

FILE 'CAPLUS, EMBASE, BIOSIS, MEDLINE, WPIDS' ENTERED AT 15:27:57 ON 27 APR 2005

C:\Program Files\Stnexp\Queries\





chain nodes :
13 14 15 16
ring nodes :
1 2 3 4 5 6 7 8 9 10
chain bonds :
3-10 5-15 8-13 13-14 15-16
ring bonds :
1-2 1-5 2-3 3-4 4-5 6-7 6-10 7-8 8-9 9-10
exact/norm bonds :
1-2 1-5 2-3 3-4 3-10 4-5 5-15 6-7 6-10 7-8 8-9
8-13 9-10 13-14 15-16

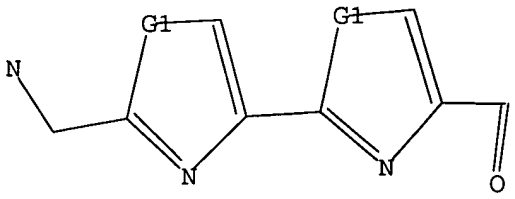
G1:O,S

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom
8:Atom 9:Atom 10:Atom 13:CLASS 14:CLASS 15:CLASS
16:CLASS

Uploading C:\Program Files\Stnexp\Queries\09936972.str

L1 STRUCTURE UPLOADED

=> d l1
L1 HAS NO ANSWERS
L1 STR



G1 O,S

Structure attributes must be viewed using STN Express query preparation.

=> s l1
SAMPLE SEARCH INITIATED 15:05:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 9 TO ITERATE

100.0% PROCESSED 9 ITERATIONS 1 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 9 TO 360
PROJECTED ANSWERS: 1 TO 80

L2 1 SEA SSS SAM L1

=> d all

L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2005 ACS on STN
RN 234125-15-6 REGISTRY
ED Entered STN: 21 Aug 1999
CN L-Isoleucine, L-valylglycyl-L-isoleucylglycylglycylglycylglycylglycylglycylglycylglycyl-2-[2-(aminomethyl)-4-oxazolyl]-4-thiazolecarbonylglycylglycyl-L-glutaminylglycylglycyl-2-(aminomethyl)-4-thiazolecarbonylglycyl-2-(aminomethyl)-4-thiazolecarbonyl-L-seryl-L-asparaginyl-2-(aminomethyl)-4-thiazolecarbonylglycylglycylglycyl-L-asparaginylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-2-(aminomethyl)-4-oxazolecarbonylglycyl-L-seryl-L-histidyl- (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
SQL 36
NTE

type	location		description
uncommon	Oaa-13	-	-
uncommon	Oaa-19	-	-
uncommon	Oaa-21	-	-
uncommon	Oaa-24	-	-
uncommon	Oaa-30	-	-
uncommon	Oaa-32	-	-

SEQ 1 VGIGGGGGGG GGXGGQGGXG XSNXGGGNGX GXGSHI

SEQ3 1 Val-Gly-Ile-Gly-Gly-Gly-Gly-Gly-Gly-Gly-
11 Gly-Gly-Oaa-Gly-Gly-Gln-Gly-Gly-Oaa-Gly-
21 Oaa-Ser-Asn-Oaa-Gly-Gly-Gly-Asn-Gly-Oaa-
31 Gly-Oaa-Gly-Ser-His-Ile

MF C117 H158 N48 O45 S4
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER
DT.CA CAplus document type: Journal
RL.NP Roles from non-patents: BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3N2	NCNC2	5	C3N2	16.195.24	1
C3NO	NCOC2	5	C3NO	16.239.9	3
C3NS	NCSC2	5	C3NS	16.299.11	4

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

AN 135:269150 CA
TI In vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bisheterocyclic sites
AU Zamble, Deborah B.; Miller, Deborah A.; Heddle, Jonathan G.; Maxwell, Anthony; Walsh, Christopher T.; Hollfelder, Florian
CS Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SO Proceedings of the National Academy of Sciences of the United States of America (2001), 98(14), 7712-7717
CODEN: PNASA6; ISSN: 0027-8424
PB National Academy of Sciences
DT Journal
LA English
CC 7-3 (Enzymes)
AB Microcin B17 (MccB17) is a 3.1-kDa Escherichia coli antibiotic that contains thiazole and oxazole heterocycles in a peptide backbone. MccB17 inhibits its cellular target, DNA gyrase, by trapping the enzyme in a complex that is covalently bound to double-strand cleaved DNA, in a manner similar to the well-known quinolone drugs. The identification of gyrase as the target of MccB17 provides an opportunity to analyze the relationship between the structure of this unusual antibiotic and its activity. In this report, steady-state parameters are used to describe the induction of the cleavable complex by MccB17 analogs containing modified bis-heterocyclic sites. The relative potency of these analogs corresponds to the capacity of the compds. to prevent growth of sensitive cells. In contrast to previously reported expts., inhibition of DNA gyrase supercoiling activity by wild-type MccB17 also was observed These results suggest that DNA gyrase is the main intracellular target of MccB17. This study probes the structure-function relationship of a new class of gyrase inhibitors and demonstrates that these techniques could be used to analyze compds. in the search for clin. useful antibiotics that block DNA gyrase.
ST DNA gyrase inhibition microcin B17 analog
IT Enzymes, biological studies
RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(DNA gyrases, A and B; in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT Structure-activity relationship
(enzyme-inhibiting, DNA gyrase-inhibiting; in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT Enzyme kinetics
Supercoiled structure
(in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
IT 84286-90-8, microcin B17 84286-90-8D, microcin B17, analogs 234125-07-6 234125-08-7 234125-11-2 234125-15-6 234125-18-9
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
(in vitro characterization of DNA gyrase inhibition by microcin B17 analogs with altered bis-heterocyclic sites)
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
(1) Bayer, A; Eur J Biochem 1995, V234, P414 CAPLUS
(2) Critchlow, S; Biochemistry 1996, V35, P7387 CAPLUS
(3) Drlica, K; Curr Opin Microbiol 1999, V2, P504 CAPLUS
(4) Drlica, K; Microbiol Mol Biol Rev 1997, V61, P377 CAPLUS
(5) Heddle, J; J Mol Biol 2001, V307, P1223 CAPLUS
(6) Herrero, M; J Gen Microbiol 1986, V132, P393 CAPLUS
(7) Hiasa, H; J Biol Chem 1996, V271, P26424 CAPLUS
(8) Hooper, D; Clin Infect Dis 1998, V27, PS54 CAPLUS
(9) Kampranis, S; J Biol Chem 1998, V273, P22615 CAPLUS
(10) Kolter, R; Annu Rev Microbiol 1992, V46, P141 CAPLUS
(11) Madison, L; Mol Microbiol 1997, V23, P161 CAPLUS
(12) Maxwell, A; Protocols of DNA Topoisomerases I: DNA Topology and Enzyme Purification 1999, P135 CAPLUS
(13) Maxwell, A; Trends Microbiol 1997, V5, P102 MEDLINE
(14) Moreno, F; Genetics and Biochemistry of Antibiotic Production 1995, P307 CAPLUS
(15) Reece, R; Crit Rev Biochem Mol Biol 1991, V26, P335 CAPLUS
(16) Roca, J; Trends Biochem Sci 1995, V20, P156 CAPLUS
(17) Shen, L; Biochemistry 1989, V28, P3879 CAPLUS
(18) Shen, L; J Biol Chem 1989, V264, P2973 CAPLUS
(19) Sinha Roy, R; Chem Biol 1999, V6, P305 MEDLINE
(20) Sinha Roy, R; Nat Prod Rep 1999, V16, P249
(21) Stubbe, J; Acc Chem Res 1996, V29, P322 CAPLUS
(22) Vizan, J; EMBO J 1991, V10, P467 CAPLUS
(23) Wentzell, L; J Mol Biol 2000, V304, P779 CAPLUS
(24) Yorgey, P; Mol Microbiol 1993, V9, P897 CAPLUS
(25) Yorgey, P; Proc Natl Acad Sci USA 1994, V91, P4519 CAPLUS
(26) Yoshida, H; Antimicrob Agents Chemother 1993, V37, P839 CAPLUS
(27) Zuber, G; J Am Chem Soc 1998, V120, P9368 CAPLUS

REFERENCE 2

AN 131:127509 CA
TI In vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites
AU Roy, Ranabir Sinha; Kelleher, Neil L.; Milne, Jill C.; Walsh, Christopher T.
CS Department of Biological Chemistry and Molecular Pharmacology, Harvard Medical School, Boston, MA, 02115, USA
SO Chemistry & Biology (1999), 6(5), 305-318
CODEN: CBOLE2; ISSN: 1074-5521
PB Current Biology Publications
DT Journal
LA English
CC 10-5 (Microbial, Algal, and Fungal Biochemistry)

AB The Escherichia coli peptide antibiotic microcin B17 (MccB17) contains 4 oxazole and 4 thiazole rings and inhibits DNA gyrase. The role of individual and tandem pairs of heterocycles in bioactivity has not been determined previously. The 2 tandem 4,2-bisheterocycles in MccB17 were varied by expression of MccB17 or mutants containing altered sequences at Gly39-Ser40-Cys41 or Gly54-Cys55-Ser56. A mixture of 5-9-ring MccB17 isoforms were separated and quantitated for antibiotic potency. Mutagenesis of the thiazole-oxazole pair significantly affected antibiotic activity compared with the upstream oxazole-thiazole, which might stabilize partially cyclized intermediates against proteolysis. Enzymic heterocyclization in native MccB17 occurs distributively. Antibiotic activity correlates with the number of rings and is differentially sensitive to both the location and the identity of the 4,2-tandem heterocycle pairs in MccB17. Such tandem heterocycles might be useful pharmacophores in combinatorial libraries.

ST antibiotic activity microcin B17 analog

IT Structure-activity relationship
(bactericidal; in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

IT Antibiotics
(in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

IT 84286-90-8DP, Microcin B17, analogs 234125-07-6P 234125-08-7P 234125-09-8P 234125-10-1P 234125-11-2P 234125-12-3P 234125-13-4P 234125-14-5P 234125-15-6P 234125-16-7P 234125-17-8P 234125-18-9P
RL: BAC (Biological activity or effector, except adverse); BPN (Biosynthetic preparation); BSU (Biological study, unclassified); BIOL (Biological study); PREP (Preparation)
(in vivo processing and antibiotic activity of microcin B17 analogs with varying ring content and altered bisheterocyclic sites)

RE.CNT 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD

(1) Asencio, C; Biochem Biophys Res Commun 1976, V69, P7
(2) Bayer, A; Eur J Biochem 1995, V234, P414 CAPLUS
(3) Belshaw, P; Chem Biol 1998, V5, P373 CAPLUS
(4) Davagnino, J; Proteins 1986, V1, P230 CAPLUS
(5) Deng, W; Anal Biochem 1992, V200, P81 CAPLUS
(6) Fenn, J; Biol Mass Spectrom 1990, V9, P37 CAPLUS
(7) Garrido, M; EMBO J 1988, V7, P1853 CAPLUS
(8) Gauthier, J; Anal Chim Acta 1991, V246, P211 CAPLUS
(9) Gellert, M; Proc Natl Acad Sci USA 1976, V73, P3872 CAPLUS
(10) Genilloud, O; J Bacteriol 1989, V171, P1126 CAPLUS
(11) Herrero, M; J Gen Microbiol 1986, V132, P393 CAPLUS
(12) Hillenkamp, F; Anal Chem 1991, V63, P1193A CAPLUS
(13) Ho, S; Gene 1989, V77, P51 CAPLUS
(14) Ichiba, T; J Am Chem Soc 1991, V113, P3173 CAPLUS
(15) Kelleher, N; J Am Chem Soc 1998, V120, P9716 CAPLUS
(16) Lavina, M; J Gen Microbiol 1986, V132, P1685 CAPLUS
(17) Li, Y; Science 1996, V274, P1188 CAPLUS
(18) Little, D; Anal Chem 1994, V66, P2809 CAPLUS
(19) Madison, L; Mol Microbiol 1997, V23, P161 CAPLUS
(20) Mayr-Harting, A; Meth Microbiol 1972, V7A, P315 CAPLUS
(21) Milne, J; Biochemistry 1998, V37, P13250 CAPLUS
(22) Moses, R; J Biol Chem 1972, V247, P6031 CAPLUS
(23) Roepstorff, P; Biomed Mass Spec 1984, V11, P601 CAPLUS
(24) San Millan, J; J Bacteriol 1985, V163, P1016 CAPLUS
(25) San Millan, J; J Bacteriol 1985, V163, P275 CAPLUS
(26) Selva, E; The J Antibiot 1997, V50, P22 CAPLUS
(27) Senko, M; J Am Soc Mass Spectrom 1995, V6, P229 CAPLUS
(28) Senko, M; Rapid Commun Mass Spectrom 1996, V10, P1824 CAPLUS
(29) Shen, L; Curr Pharm Des 1996, V2, P195 CAPLUS
(30) Sinha, R; Biochemistry 1998, V37, P4125
(31) Sinha, R; Chem Biol 1998, V5, P217

(32) Takita, T; J Antibiot 1978, V31, P801 CAPLUS
(33) Vanderwall, D; Chem Biol 1997, V4, P373 CAPLUS
(34) Vizan, J; EMBO J 1991, V10, P467 CAPLUS
(35) Wilm, M; Anal Chem 1996, V68, P1 CAPLUS
(36) Yorgey, P; Mol Microbiol 1993, V9, P897 CAPLUS
(37) Yorgey, P; PhD Thesis Harvard University 1993
(38) Yorgey, P; Proc Natl Acad Sci USA 1994, V91, P4519 CAPLUS
(39) Zuber, G; J Am Chem Soc 1998, V120, P9368 CAPLUS

=>

L13 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1996:639425 CAPLUS
DN 125:329404
TI Synthesis of all-**thiazole** microcin B17
AU Videnov, G.; Ihlenfeldt, H. G.; Bayer, A.; **Jung, G.**
CS Institut fur Organische Chemie, Universitat Tubingen, Tuebingen, D-72076, Germany
SO Peptides 1994, Proceedings of the European Peptide Symposium, 23rd, Braga, Port., Sept. 4-10, 1994 (1995), Meeting Date 1994, 351-352. Editor(s): Maia, Hernani L. S. Publisher: ESCOM, Leiden, Neth.
CODEN: 63MBAO
DT Conference
LA English

L13 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:288460 CAPLUS
DN 133:4987
ED Entered STN: 04 May 2000
TI Synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides, cyclotetrapeptide and their antibacterial activity in vitro
AU Stankova, Ivanka G.; Videnov, Georgi I.; Tabakova, Svoboda; Golovinsky, Evgeny V.; **Jung, Guenther**
CS Department of Chemistry, South - West University "N. Rilski", Blagoevgrad, 2700, Bulg.
SO Peptides 1998, Proceedings of the European Peptide Symposium, 25th, Budapest, Aug. 30-Sept. 4, 1998 (1999), Meeting Date 1998, 248-249. Editor(s): Bajusz, Sandor; Hudecz, Ferenc. Publisher: Akademiai Kiado, Budapest, Hung.
CODEN: 68WKAY
DT Conference
LA English
CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 10, 28
AB A symposium report. We describe the synthesis and antibacterial activity of new peptides and a cyclopeptide containing imidazole, **thiazole** and **oxazole** rings. Two compds. were active against Staphylococcus, Klebsiella and Streptococcus strains.
ST peptide imidazole **thiazole** **oxazole** ring prepn antibacterial symposium
IT Antibacterial agents
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
IT Peptides, preparation
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
IT 270908-01-5P 270908-02-6P 270908-03-7P 270908-04-8P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(synthesis of novel imidazole, **thiazole**, **oxazole** substituted peptides and a cyclotetrapeptide and their antibacterial activity in vitro)
RE.CNT 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE
(1) Bergeron, J; J Org Chem 1985, V50, P2780
(2) Fusetani, N; Chem Rev 1993, V93, P1793 CAPLUS
(3) Jones, C; Tetrahedron Lett 1988, V29, P3851
(4) Reiner, R; Antibiotic 1982, P21
(5) Videnov, G; Angew Chem 1996, V108, P1604
(6) Videnov, G; Angew Chem Int Ed Engl 1996, V35, P1503 CAPLUS